Computational Science and Engineering Education: Breaking the Disciplinary Barriers

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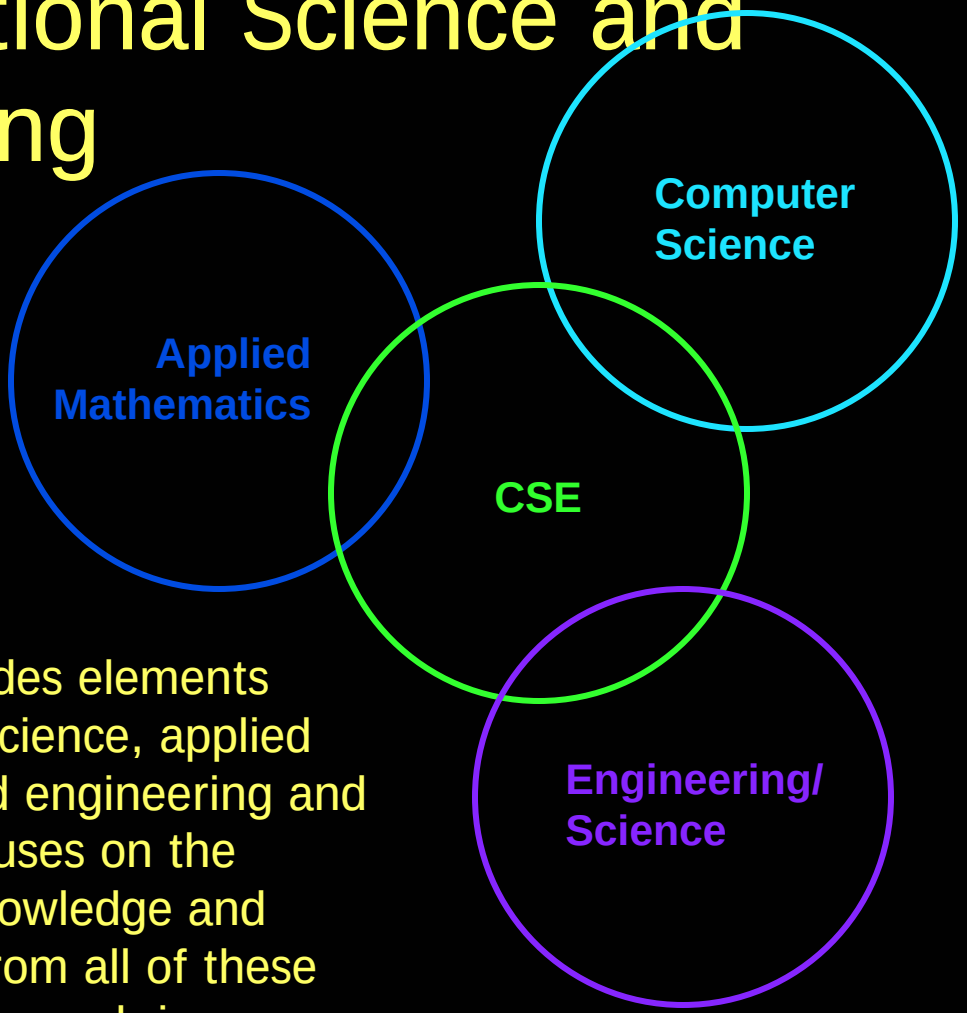
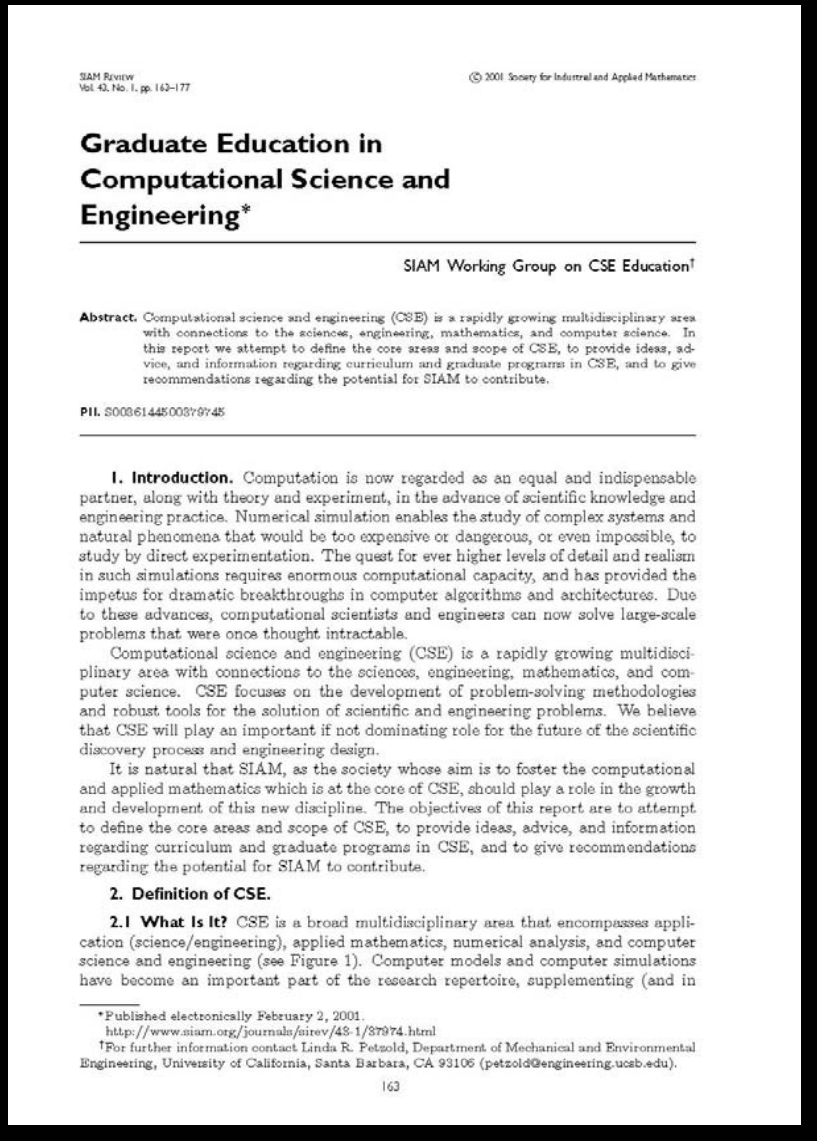
Computational Science and Engineering



Although it includes elements from computer science, applied mathematics and engineering and science, CSE focuses on the *integration* of knowledge and methodologies from all of these disciplines, and as such is a subject which is distinct from any of them.

SIAM Report on CSE Graduate Education, 2000

- Outlined the core components for CSE graduate programs
- Highlighted several programs with different structures



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Graduate Education in Computational Science and Engineering*

SIAM Working Group on CSE Education†

Abstract. Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics, and computer science. In this report we attempt to define the core areas and scope of CSE, to provide ideas, advice, and information regarding curriculum and graduate programs in CSE, and to give recommendations regarding the potential for SIAM to contribute.

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1. Introduction. Computation is now regarded as an equal and indispensable partner, along with theory and experiment, in the advance of scientific knowledge and engineering practice. Numerical simulation enables the study of complex systems and natural phenomena that would be too expensive or dangerous, or even impossible, to study by direct experimentation. The quest for ever higher levels of detail and realism in such simulations requires enormous computational capacity, and has provided the impetus for dramatic breakthroughs in computer algorithms and architectures. Due to these advances, computational scientists and engineers can now solve large-scale problems that were once thought intractable.

Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, mathematics, and computer science. CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design.

It is natural that SIAM, as the society whose aim is to foster the computational and applied mathematics which is at the core of CSE, should play a role in the growth and development of this new discipline. The objectives of this report are to attempt to define the core areas and scope of CSE, to provide ideas, advice, and information regarding curriculum and graduate programs in CSE, and to give recommendations regarding the potential for SIAM to contribute.

2. Definition of CSE.

2.1 What Is It? CSE is a broad multidisciplinary area that encompasses application (science/engineering), applied mathematics, numerical analysis, and computer science and engineering (see Figure 1). Computer models and computer simulations have become an important part of the research repertoire, supplementing (and in

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Models for CSE Graduate Education

Department or Program

- + Fits within traditional University structure: Resources are available for administrative support, TAs and fellowships, space
- - Are students getting enough depth in science and engineering areas? Are faculty in S&E an integral part of the program?
- - Job market for CSE degree is not well documented or tested, particularly for students wanting to pursue academic careers

Cross-Disciplinary Emphasis

- + Ensures depth in a traditional discipline
- + Job market is well-established
- + Provides a multidisciplinary structure within the University that can be built upon for both research and education
- - Cuts across traditional University structure: Resources are not easily available within the University

CSE Graduate Programs Today

- **Department:**

  SUNY Brockport (MS)

- **Graduate Degree:**

  George Mason (MS), Mississippi State, Rice , San Diego State/Claremont, Stanford, Minnesota, MIT (MS), Louisiana Tech, UT Austin

- **Graduate Emphasis:**

  Boston U., George Washington , Purdue, RPI, Syracuse, UCSB, U. of Houston, Illinois Urbana, Maryland College Park, Michigan, Southern Mississippi, Utah, William and Mary, Wayne State, Florida State, Duke, Indiana, Stanford, Clemson, Arizona, Clarkson

- **CSE Track:**

  many, mostly in math or CS departments

UCSB Graduate Emphasis in CSE

MS or PhD in traditional discipline, with specialization in CSE

- Mechanical and Environmental Engineering
- Computer Science
- Mathematics
- Chemical Engineering
- Electrical and Computer Engineering
- Geology

Core CSE courses *(most cross-listed across all departments)*

- Two quarters applied mathematics sequence
- Four quarters numerical computation sequence
  (students must take at least three quarters)
- One quarter parallel computation

Overall load is the same as for students without the specialization

Initial creation of program: 2 years effort, talk to many faculty, negotiate program requirements with the Departments. Helpful to be in multiple departments. Necessary: administration buy-in, release time, secretarial support, website development support, grad student support

UCSB IGERT Program in CSE

NSF IGERT: Integrative Graduate Education Research Traineeship program - $2.9 million/5 years

PhD Program, 2 years guaranteed support

- (fellowships are limited by NSF to US Citizens and permanent residents, but the educational program is open to all via IGERT Associate Program)

Departments:

- Chemical Engineering, Computer Science, Mathematics, Mechanical and Environmental Engineering

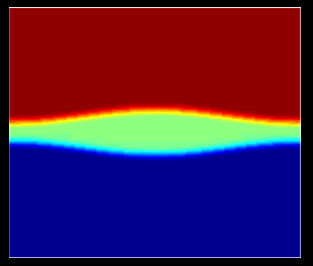
Research: Focus on multiscale problems. Students and faculty work in multidisciplinary teams. Theses are jointly supervised from 2 Departments.

- Complex Fluids
- Computational Materials
- Microscale Engineering
- Computational Systems Biology

Internship

Career development workshop, guest speakers and visitors, travel support

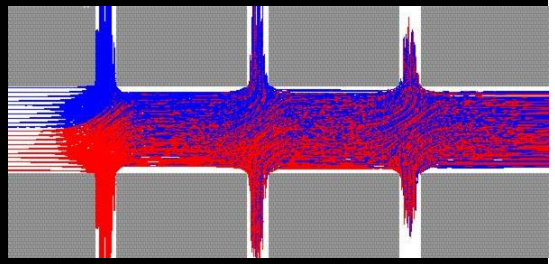
IGERT Focus Groups



Evolution of temperature distribution in thermal convection

Complex Fluids

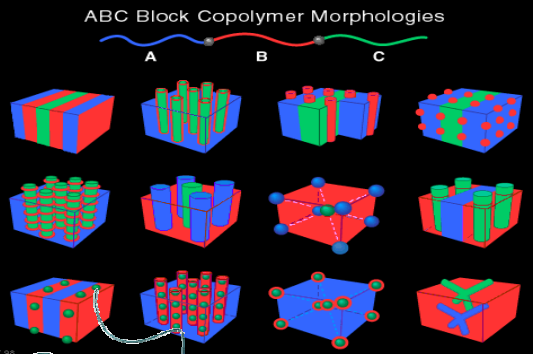
- Field-theoretic computer simulations
- Korteweg stresses in miscible fluid flows
- Liquid crystalline polymers in flow
- Dynamics of entangled polymers in flow



Micromixer

Microscale Engineering

- Mixing in microchannels
- Microfluidics
- Electrokinetic phenomena

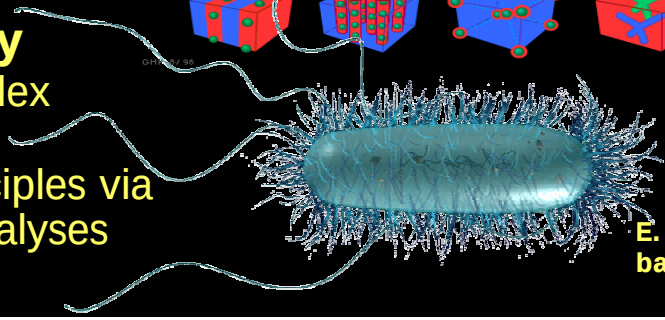


Computational Materials

- Ferroelectric ceramics
- Ceramic composites

Computational Systems Biology

- Multi-scale simulation of complex biochemical networks
- Unraveling robust design principles via sensitivity and robustness analyses

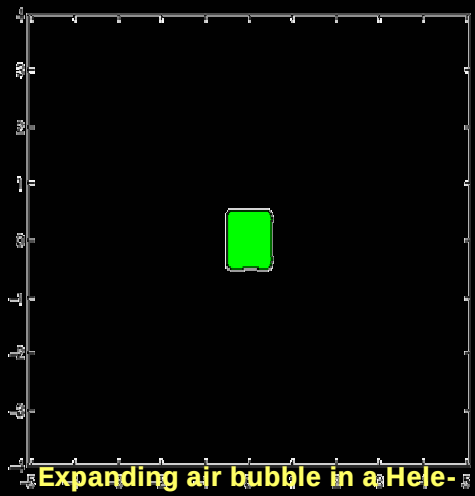


E. coli bacterium

IGERT Enabling Technologies

Computational and Applied Mathematics

- Multiscale simulation methods for chemical kinetic systems
- Stochastic partial differential equations
- Homogenization
- Sharp gradients and interface tracking
- Computational analysis tools for multiscale systems



Expanding air bubble in a Hele-Shaw flow with surface tension

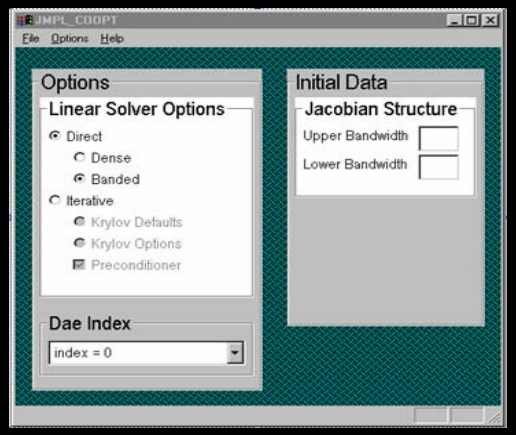
Computer Science

- Semi-automatic generation of graphical user interfaces for scientific computing
- Cluster computing and grid computing environments

NETWORK WEATHER SERVICE

Monitor and forecast performance of network and computational resources

JMPL (Java Math Package Launcher)



UCSB IGERT Program in CSE

We are in the second year of a 5-year program

- 11 fellows:
  - 7 male
  - 4 female
- 6 associates:
  - 4 male
  - 2 female

Biggest Success:

Multidisciplinary research teams - *building research teams from the ground up*

- Modeled after multidisciplinary research teams in Laboratories and industry.
- Spawns new multidisciplinary research collaborations and strengthens existing ones.
- Exciting, collaborative environment attracts students, postdocs and faculty who may not even be directly funded by the Program.
- Most students find it overwhelming at first but rapidly rise to the challenge.

Resources: *What do we have?*

Multidisciplinary Graduate Training:

- NSF IGERT - *highly competitive program, funds CSE programs at UCSB, Boston U.*

Graduate Fellowships:

- DOE Computational Science Graduate Fellowships –*funds a limited number of students scattered across the US*

DOE Laboratories:

- Student internships
- Summer programs
- Engage faculty

Multidisciplinary CSE Research Support:

- NSF ITR - *widely influential in enabling multidisciplinary research in the academic community. What's next???*
- DOE SCIDAC - *connection to DOE Laboratories*

Resources: *What do we need?*

Funding that can be leveraged to build programs:

- Integration of research and education.
- NSF IGERT is a good model, but can fund very few CSE programs.
- Find out what works and fund programs that pursue those paths. Monitor progress.
- Administrative support personnel, computer resources, PI teaching release are essential.

Well-designed multidisciplinary research funding:

- Coordination between agencies: NSF, DOE, NIH.
- Seamless access to supercomputing resources.
- Educational objectives for large research grants should foster multidisciplinary collaboration: research in teams, joint thesis advising… Judge by track record, integration with the research plan, not necessarily by innovation.

A home in the NSF for Multidisciplinary CSE:

- ITR is disappearing!!!
- NSF cross-cutting programs have been highly influential in restructuring the way research is done at the University.
- There are no cross-cutting disciplines within the NSF structure. There is no stable long-term funding base for cross-cutting disciplines.
- To restructure the University, provide the new structure within the NSF.